

Calculations Used in Analytical Chemistry

Chapter 4

Slide 1

Topics

- International System of Units / SI Units
- Mass and Weight
- The Mole
- Units of Concentrations of solutions
- Stoichiometry

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Seven SI BASE UNITS

TABLE 4-1

SI Base Units		
Physical Quantity	Name of Unit	Abbreviation
Mass	kilogram	kg
Length	meter	m
Time	second	s
Temperature	kelvin	K
Amount of substance	mole	mol
Electric current	ampere	A
Luminous intensity	candela	cd

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Derived units:

All other units can be derived from the seven base units

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Table 4-1, p.72

Examples of Derived Units

- 1 Joule=?
- 1 Newton=?
- 1 volt=?

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TABLE 4-2

Prefixes for Units

Prefix	Abbreviation	Multiplier
yotta-	Y	10^{24}
zetta-	Z	10^{21}
exa-	E	10^{18}
peta-	P	10^{15}
tera-	T	10^{12}
giga-	G	10^9
mega-	M	10^6
kilo-	k	10^3
hecto-	h	10^2
deca-	da	10^1
deci-	d	10^{-1}
centi-	c	10^{-2}
milli-	m	10^{-3}
micro-	μ	10^{-6}
nano-	n	10^{-9}
pico-	p	10^{-12}
femto-	f	10^{-15}
atto-	a	10^{-18}
zepto-	z	10^{-21}
yocto-	y	10^{-24}

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Table 4-1, p.72

Mass and Weight

- Mass (m): invariant measure of amount of matter
- Weight

$$W = mg$$

- g: acceleration due to gravity



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Calculating moles from mass Factor Label Method Review

- Mass of TRIS that will react with 35 mL of 0.1 M HCl.

- Moles of HCl in 35 mL

$$\text{mol HCl} = V_{\text{HCl}} \times M_{\text{HCl}} =$$

- Moles of TRIS

$$n_{\text{TRIS}} = \# \text{mol HCl} \times \frac{1 \text{ mol TRIS}}{1 \text{ mol HCl}}$$

- Mass of TRIS

mol TRIS x molar mass TRIS

$$m_{\text{TRIS}} = \# \text{mol TRIS} \times \frac{121.14 \text{ g TRIS}}{1 \text{ mol TRIS}}$$

Use the factor label method : Prelab of Experiment 3

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The Mole

- Mole (mol): SI unit for the amount of a chemical species
- 1 mole = 6.022×10^{23} particles
- Molar mass: mass (in g) of one mole
- Calculating molar masses using EXCEL (Chapter 3, p 60-67).
 - Importing data from Web Pages
 - Dealing with Character Strings (FIND function, MID function)
 - Using VLOOKUP to locate Data in a Worksheet



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Solutions and their Concentrations

- Analytical molarity
- Equilibrium molarity
- Percent concentration
- Parts per Million/Billion
- P-Functions or p-value

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Solutions and their Concentrations

- Analytical molarity
 - Total number of moles of a solute in 1L of the solution (according to recipe).Example: NaCl, Na₂SO₄
- Equilibrium molarity
 - Molar concentration of a given species in solution

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Percent Concentrations

$$\text{weight} - \text{percent} - (w/w) = \frac{\text{weight} - \text{solute}}{\text{weight} - \text{solution}} \times 100\%$$

$$\text{Volume} - \text{percent} - (V/V) = \frac{\text{volume} - \text{solute}}{\text{volume} - \text{solution}} \times 100\%$$

$$\text{weight} / \text{volume} - \text{percent} - (w/v) = \frac{\text{weight} - \text{solute}, g}{\text{volume} - \text{solution}, mL} \times 100\%$$

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2.5 L **9535-03**
Hydrochloric Acid,
36.5-38.0%
 Acide Hydrochlorique
'BAKER ANALYZED'® A.C.S. Reagent
HCl **FW 36.46**
LOT

Meets A.C.S. Specifications
 Meets Reagent Specifications for testing USP/NF monographs
 Appearance Passes Test
 Assay (as HCl) (by acid-base titm) 36.5 - 38.0 %
 Color (APHA) 10 max.
 Extractable Organic Substances 5 ppm max.
 Free Chlorine (as Cl) 1 ppm max.
 Residue after Ignition 3 ppm max.
 Specific Gravity at 60°/60°F 1.185 - 1.192
 Bromide (Br) 0.005 % max.
 Trace Impurities (in ppm):
 Phosphate (PO₄) 1 max.
 Sulfate (SO₄) 0.5 max.
 Sulfite (SO₃) 0.8 max.
 Ammonium (NH₄) 3 max.
 Trace Impurities (in ppb):
 Aluminum (Al) 100 max.
 Arsenic and Antimony (as As) 5 max.
 Boron (B) 50 max.
 Calcium (Ca) 200 max.
 Chromium (Cr) 100 max.
 Copper (Cu) 100 max.
 Gold (Au) 100 max.
 Heavy Metals (as Pb) 100 max.
 Iron (Fe) 100 max.
 Lead (Pb) 50 max.
 Magnesium (Mg) 300 max.
 Manganese (Mn) 300 max.
 Mercury (Hg) 5 max.
 Nickel (Ni) 100 max.
 Potassium (K) 300 max.
 Sodium (Na) 300 max.
 Tin (Sn) 300 max.
 Titanium (Ti) 300 max.
 Zinc (Zn) 100 max.
 Water CAS No: 7732-18-5
 Hydrogen Chloride CAS No: 7647-01-0

SAF-T-DATA™ System

HEALTH	FLAMMABILITY	REACTIVITY	CONTACT
3	0	2	3
SEVERE	NONE	MODERATE	SEVERE

LABORATORY PROTECTIVE EQUIPMENT

GOGGLES & SHIELD	LAB COAT & APRON	VENT HOOD	PROPER GLOVES
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STORAGE COLOR: WHITE

DOT Name: HYDROCHLORIC ACID
UN1789

CAS NO: 7647-01-0

J. T. Baker NEUTRASORB® or TEAM® Low Na⁺ acid neutralizers are recommended for spills of this product.

MADE IN USA



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Fig 4-1, p.82

Density and Specific Gravity of Solutions

- Density of a substance is its mass per unit volume
- Specific gravity: ratio of mass of substance to the mass of equal volume of water at 4°C.
- When using the metric system density and specific gravity can be used interchangeably, because the density of water is approximately 1.00 g/mL

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From % w/w to mol/L solution

- 36.5 % HCl
- FW = 36.46
- Specific gravity = 1.18

$$c_{HCl} = \frac{mol}{L \text{ soln}} = 36.5 g_{HCl} \times \frac{1 mol_{HCl}}{36.46 g_{HCl}} \times \frac{1}{100 g \text{ soln}} \times \frac{1.18 g}{1.00 mL} \times \frac{1000 mL}{1 L} \approx 11.8 M$$

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TABLE 4-3

Specific Gravities of Commercial Concentrated Acids and Bases

Reagent	Concentration, % (w/w)	Specific Gravity
Acetic acid	99.7	1.05
Ammonia	29.0	0.90
Hydrochloric acid	37.2	1.19
Hydrofluoric acid	49.5	1.15
Nitric acid	70.5	1.42
Perchloric acid	71.0	1.67
Phosphoric acid	86.0	1.71
Sulfuric acid	96.5	1.84

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Table 4-3, p.82

Back to Concentrations: Parts Per Million, Parts per Billion

- For very dilute solutions, it is convenient to express concentrations in ppm or ppb
- An approximation that is commonly used is that the density of dilute solution approaches the density of water (1.00 g/ml)

$$c_{ppm} = \frac{\text{mass} - \text{solute}}{\text{mass} - \text{solution}} \times 10^6 \text{ ppm}$$

$$c_{ppb} = \frac{\text{mass} - \text{solute}}{\text{mass} - \text{solution}} \times 10^9 \text{ ppb}$$

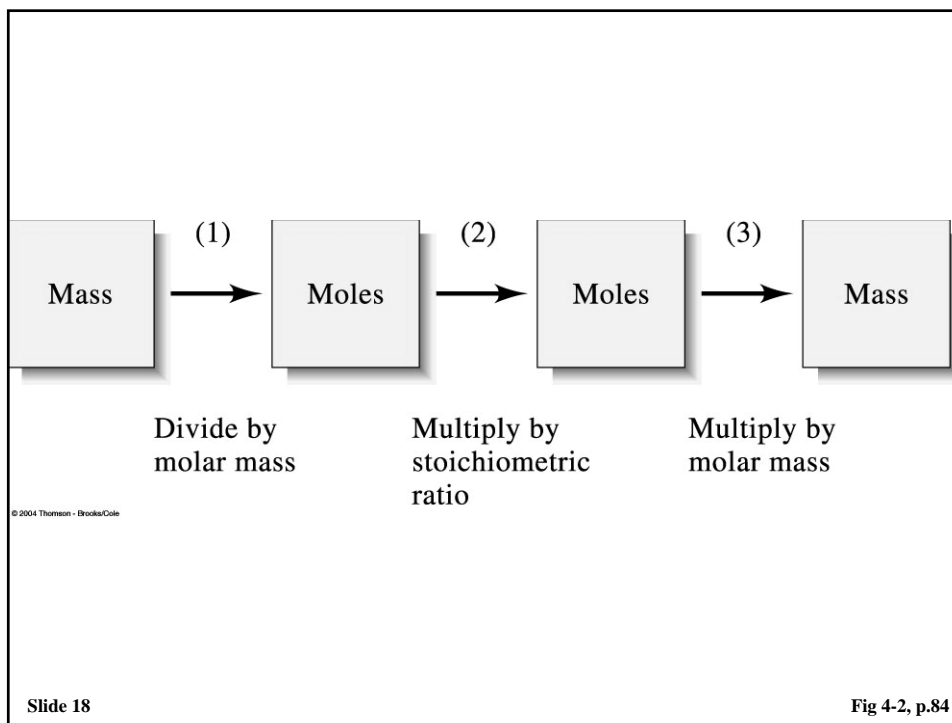
Units in numerator and denominator must be consistent!

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Back to Concentrations: p-functions or p-values

- The p-value is the negative log (base 10) of the molar concentration
- P-values are convenient to use when changes occur over several orders of magnitude
- $[H^+]$, pH
- $[Ba^{2+}]$, pBa
- $[Cl^-]$, pCl
- $[Cl^-] = 2.45 \times 10^{-5} M$
 $pCl = 4.6108 = 4.61?$

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Stoichiometric Calculations

- Problem 4-36
 - What mass of MgNH_4PO_4 precipitated when 200.00 mL of a 1.000% (w/v) solution of MgCl_2 were treated with 40.0 mL of 0.1753 M Na_3PO_4 and an excess of NH_4^+ ? What was the molarity of the excess reagent (Na_3PO_4 or MgCl_2) after the precipitation was complete?
- Steps
 - Write chemical equation and balance it
 - Calculate moles of reagents mixed
 - Determine the limiting reagent
 - Calculate mass of precipitate
 - Calculate moles of unreacted reagent
 - Calculate concentration of unreacted reagent

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Stoichiometry

- Problem 4-6:
- How many K ions are contained in 6.76 mol of K_3PO_4 ?
- $1.22 \times 10^{25} \text{ K}^+$.

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Dilution Factors

- Problem 4-30
- Describe the preparation of 1.50 mL of 0.215 M NaOH from the concentrated commercial reagent [50% NaOH (w/w)]. Specific gravity = 1.525
- 50 % NaOH (w/w) = 19.06 M
- Volume NaOH 50% (w/w) required = 16.9 mL

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